LA-UR-99-5468

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

TITLE: AIR AND WATER QUALITY MODELING SYSTEM: APPLICATION TO THE LOS ANGELES METROPOLITAN AREA

AUTHOR(S): MICHAEL J. BROWN, STEVEN J. BURIAN, TIMOTHY N. MCPHERSON, GERALD E. STREIT, KEELEY R. COSTIGAN, H. JAKE TURIN

SUBMITTED TO: 11th JOINT AMS-AWMA CONF. ON APPLICATIONS OF AIR POLLUTION METEOROLOGY LONG BEACH, CA, JAN. 2000

By acceptance of this article, the publisher recognized that the U S Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution or to allow others to do so for U S Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U S Department of Energy.

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

5.1

AIR AND WATER QUALITY MODELING SYSTEM: APPLICATION TO THE LOS ANGELES METROPOLITAN AREA

Michael Brown, Steven Burian, Timothy McPherson, Gerald Streit, Keeley Costigan, Jake Turin
Los Alamos National Laboratory, Los Alamos, New Mexico

1. INTRODUCTION

Numerical simulations from a comprehensive modeling framework for the urban air and water environment are presented. The framework is composed of air chemistry (CIT), meteorology (RAMS and HOTMAC), stormwater runoff and quality (SWMM), and receiving-water quality (WASP5) computer codes. We have simulated the transport and fate of nitrogen-containing pollutants through air and water pathways in the Los Angeles urban area. We are focusing on the transport and fate of nitrogen species because 1) they track through both air and water pathways, 2) the physics, chemistry, and biology of the complete cycle is not well understood, and 3) they have important health, local ecosystem, and global climate implications.

In this paper we give a brief overview of the models in the urban air and water modeling framework, describe results from each of the models, and present an application of the modeling system to a simplified problem in the urban environment that requires multi-disciplinary modeling. We will compare estimates of nitrogen mass fluxes to the Santa Monica Bay from runoff of atmospherically-deposited material onto the land surface and deposition directly to the bay. The framework is shown to have promise for evaluating the effects of air quality management policy on water quality management.

2. BACKGROUND

The air-water quality modeling system is applied to the transport of nitrogen species in the greater Los Angeles metropolitan region. Several of the water bodies adjacent to Los Angeles have significantly elevated levels of pollutants (SMBRP, 1998). Elevated concentrations of nutrients, metals, and organic contaminants have been found (Suffet et al., 1993; Wong et al., 1997). Although urbanization of the LA basin is certainly responsible for much of the poor water quality, it is not certain exactly what sources are the major contributors. Similar to the initial phases of the Chesapeake Bay study (Jordan et al., 1991 and Fischer and Oppenheimer, 1997), it is not clear how significant atmospheric deposition is to the water quality problem. Several large-scale air quality studies in the Los Angeles basin have shown elevated levels of particulate pollution, including nitrates (e.g., Lawson, 1990, Russell et al., 1993, Solomon et al., 1992). With the modeling system described below, we will attempt to quantify the atmospheric contribution to the water quality problem and investigate the impacts of a hypothetical emissions inventory reduction strategy.

3. MODEL DESCRIPTIONS AND SET-UP

The system of models for studying the fate of pollutants through air and water pathways is shown in Fig. 1. In short, RAMS (Pielke et al., 1992) and HOTMAC (Yamada and Kao, 1986) will provide time-dependent 3-d meteorological fields to the CIT air chemistry code (McRae et al. 1982 and Russell et al. 1988) for wet and dry season cases, respectively. CIT simulates the gas and aerosol phase chemistry and produces wet and dry deposition fields of various pollutants. The deposited pollutants were input to the SWMM model (Huber and Dickinson, 1988) along with precipitation fields from RAMS. SWMM computes urban runoff flow amounts and pollutant loading, which have been utilized by the WASP5 model (Ambrose et al., 1993) to simulate the fate of pollutants in a receiving water body. We refer interested readers to the citations above and our earlier paper (Brown et al., 1998) for descriptions of each model.

For the wet weather simulations, RAMS was run in non-hydrostatic mode and accounted for precipitation using a partial two moment microphysics scheme which includes eight water species. A nested grid approach using horizontal grid spacings of 80, 20, 5 and 1.25 km was used in order to cover the synoptic scale weather over the Pacific Ocean and Western US and to resolve the region of interest (see Costigan, 1998). For the dry weather simulations, HOTMAC was run in hydrostatic mode and used an urban canopy parameterization to account for the effect of sub-

Corresponding Author Address: Michael Brown, LANL, Group TSA-4, MS-F604, Los Alamos, NM, 87545; e-mail: mbrown@lanl.gov.

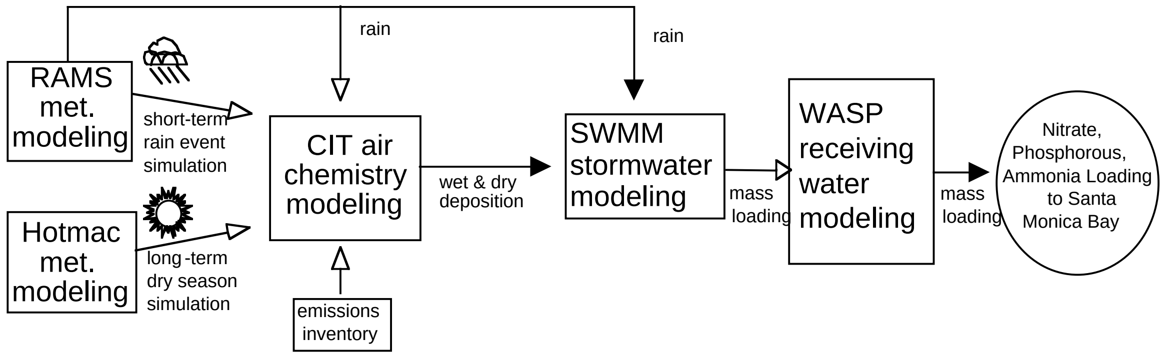

Figure 1. Modeling system for following pollutants through air-water pathways in an urban environment. With some modifications, the fate of pollutants from other sources could be modeled as well, for example, accidental releases of toxic agents, heavy metals from brake pads, or noxious vapors from waste sites.

grid buildings. A 15, 5, and 1.67 km nested grid scheme was used. The outer-most grid covers the lower 1/3 of California, the intermediate grid matches the CIT air chemistry domain, and the inner-most grid is centered over Santa Monica Bay.

CIT was applied to the Los Angeles basin for calculation of deposition of nitrogen-containing species for two periods during the 1987 Southern California Air Quality Study (SCAQS). The dry season simulation was run for August, 1987 and used the SCAQS emission inventory. The wet season simulation was for an early December, 1987 episode in which high nitrate concentrations were noted. For both cases, the CIT model was run using a single grid mesh with 5 km resolution. The modeling domain covered 24,000 km^2 and was centered over the 1,725 km^2 Santa Monica Bay watershed. The LCC chemical kinetics scheme was utilized and dry deposition was computed using the surface resistance method.

SWMM was set up to simulate the Ballona Creek watershed, a 300 km^2 heavily urbanized region of Los Angeles within the Santa Monica Bay watershed. The Ballona Creek watershed is comprised of three drainage catchments (Ballona Creek, Sepulveda Channel, and Centinela Creek) that drain into Ballona Creek, a channelized river that empties into the Santa Monica Bay. To construct the models, we digitized 2,899 storm drains from microfiche as-built drawings into a GIS environment. We also delineated 1,897 sub-catchments based on topography and drainage patterns. The SWMM RUNOFF Block was used to simulate stormwater runoff quantity and quality from the subcatchments. The RUNOFF Block implements a nonlinear reservoir algorithm to simulate runoff, while a number of water quality routines (e.g. buildup/washoff, rating curve, constant concentration) can be used to simulate the concentration of contaminants in the runoff. We inserted the accumulated deposition from the CIT model into SWMM to replace the SWMM pollutant buildup algorithm. The accumulated load is then washed off using the SWMM first-order washoff algorithm. We used the SWMM TRANSPORT Block to simulate flow and contaminant transport through the storm drainage system. The TRANSPORT Block takes the RUNOFF Block output and routes the flow and pollutants to the watershed outlet using the kinematic wave approximation to the St. Venant equations.

Surface water transport was simulated by WASP5 for the downstream end of Ballona Creek. The creek was divided into 13 segments that were 325-375 meters in length. In this study, WASP5 simulated tidally-influenced advection, dispersion, and reaction in the surface water with the DYNHYD5 hydrodynamic subroutine providing flows, depths and velocities. DYNHYD5 is connected to EUTRO5, a eutrophication kinetics module within WASP5. EUTRO5 was used to compute the concentrations of nutrients and phytoplankton and their effects on the dissolved oxygen balance. The interactions among four systems were included: phytoplankton kinetics, the phosphorus cycle, the nitrogen cycle and the dissolved oxygen balance. Reaction coefficients for the state variables were drawn from the literature (Bowie et al., 1985).

4. RESULTS

In this section, we describe results from model simulations and where appropriate describe linking

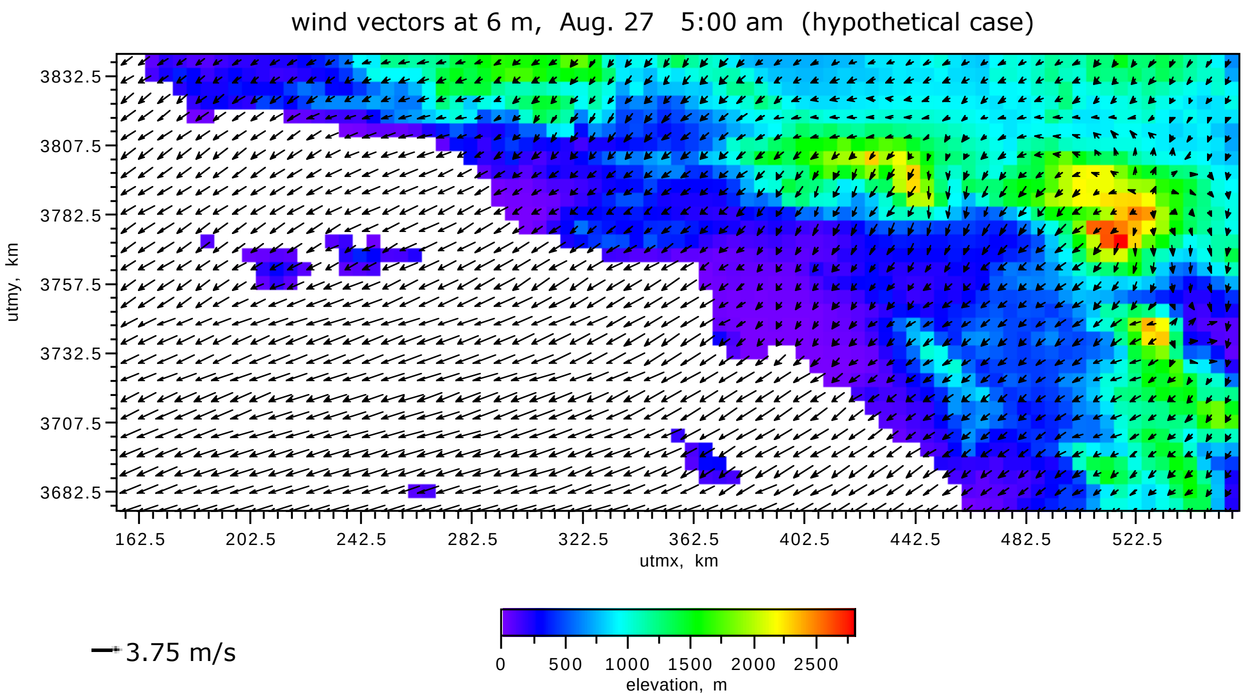

Figure 2. Wind field produced by the HOTMAC mesoscale model on the intermediate grid for prescribed easterly flow boundary conditions.

issues. We then present a case study that examines both air and water quality issues simultaneously by looking at a hypothetical air quality emissions inventory reduction strategy.

4.1 Model Results

Figure 2 shows a HOTMAC-produced wind field near the surface at 5:00 am on Aug. 27. This simulation was started at 10 pm the day before and used a Burbank rawinsonde profile to prescribe relative humidity and temperature initial conditions. The surface-level winds show mountain drainage winds interacting with the synoptically-driven winds. Some evidence of flow channeling can be seen in the mountain passes and valleys. Wind speed reduction is apparent over the Los Angeles urban area due to the urban canopy drag parameterizations included in the model physics. Speed up of the winds over the ocean results from smaller surface roughness and land-breeze induced winds.

RAMS simulations were performed for a December 4-5, 1987 precipitation event. The RAMS simulations were initialized and nudged with NCEP 2.5 degree gridded re-analysis data. Figure 3 shows the accumulated precipitation field on the fourth grid, which focuses on the LA metropolitan area with 1.25 km horizontal grid

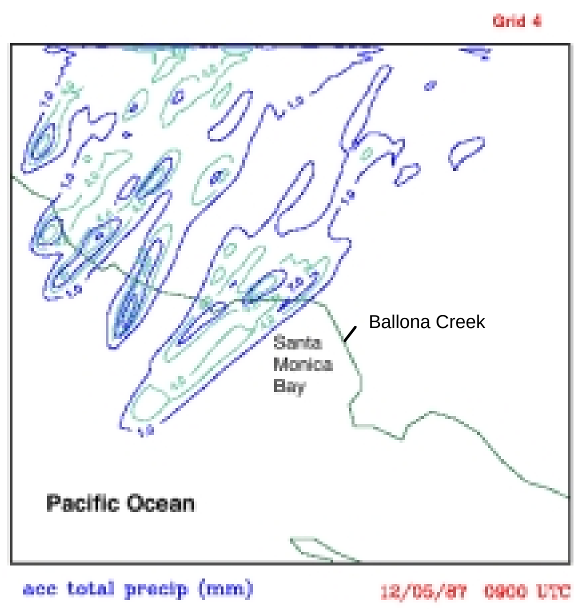

Figure 3. Contours of accumulated precipitation on the surface computed by RAMS at 1:00 am on December 5th.

spacing. The observations of precipitation in the area were somewhat greater than the model predictions of the total precipitation. This may be due to inadequate resolution of the initial meteorological fields with the reanalysis data. We

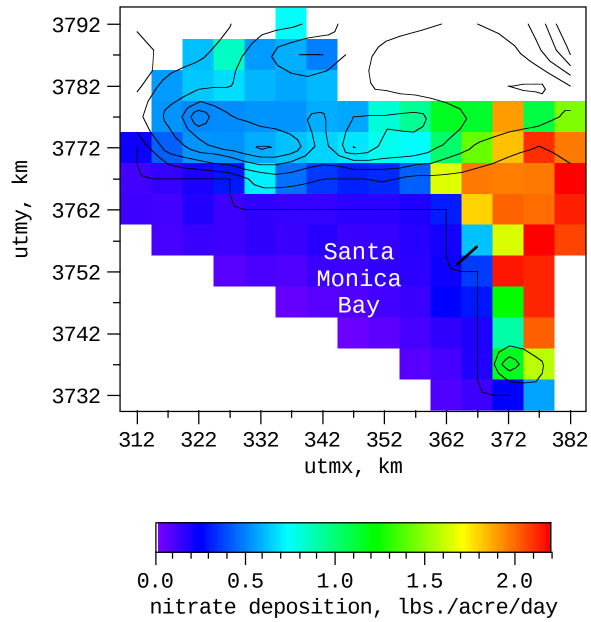

Figure 4. Nitrate deposition computed by the CIT model over the Santa Monica Bay watershed for Dec. 3, 1987. Terrain is indicated by contours.

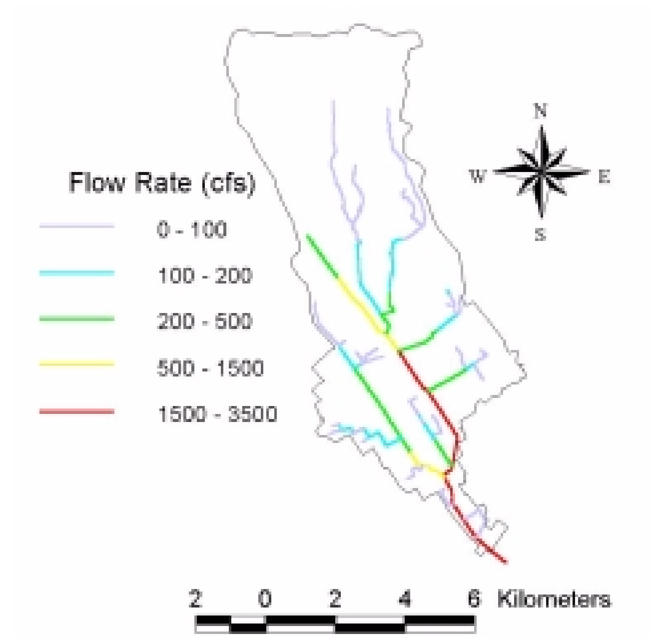

Figure 5. Flow rate computed by the SWMM model in the Sepulveda sub-catchment storm-sewer network at 5 pm on Dec. 4, 1987 three hours after the start of the rain event.

are currently adding rawinsonde observations to the initial fields and also plan to use observed sea surface temperatures (instead of climatological means) in hopes of improving the model predictions.

Although it is our intent to eventually use the HOTMAC and RAMS 3-d meteorological fields as input to the CIT model, the CIT results presented here have utilized measured winds. Once the model-computed meteorological fields have been validated and appropriate preprocessors have been finalized, we will rerun the CIT simulations incorporating this data.

Using the 1987 emissions inventory, CIT was used to compute dry deposition fields for nitrogen species for August and December time periods. Figure 4 shows the 24-hour accumulated nitrate deposition in the Santa Monica Bay watershed for Dec. 3rd, 1987. Dry deposition flux is large over the urban area, while that over the Bay is relatively small due to lower air concentrations and smaller deposition velocities over water. In comparison, the Aug. 27th period had relatively low deposition values with a maximum deposition flux of 0.7 lbs/acre/day over the urban area. Wet deposition was crudely estimated by assuming that the rainfall removed all the nitrogen-containing species in the air column.

As outlined in Burian et al. (2000), the dry and wet deposition fluxes are used as input to SWMM, although the dry deposition flux to the land surface was first corrected for plant uptake and other processes that would make it unavailable for runoff. Using 3 rainfall gauges situated in the Ballona Creek subwatershed, urban runoff from each sub-catchment was computed and then routed into the storm-sewer network. Figure 5 shows the flow rate throughout the Sepulveda sub-catchment storm drainage system shortly after the start of the Dec. 4 rainfall event. Although the flow rate naturally increases with downstream distance, one can see a decrease in flow in one of the pipes that was caused by surcharging (capacity of pipe is exceeded). Similar plots were obtained for each pollutant constituent.

The SWMM-computed flow rate and pollutant mass flux at the beginning of the Ballona Creek estuary were then incorporated into WASP5 as an upstream boundary condition. For comparison, a dry-weather flow condition was simulated as well using an existing water quality database (Stenstrom, 1999) and USGS/LADPW flow records from a flow gauging station located upstream of the estuary. Tide heights at the downstream boundary were obtained from the NOAA-COOPS database. Figure 6 indicates the effect of the storm flow on the depths and concentrations of dissolved oxygen and chlorophyll a in a segment of the Ballona Creek Estuary. The storm flow considerably altered the

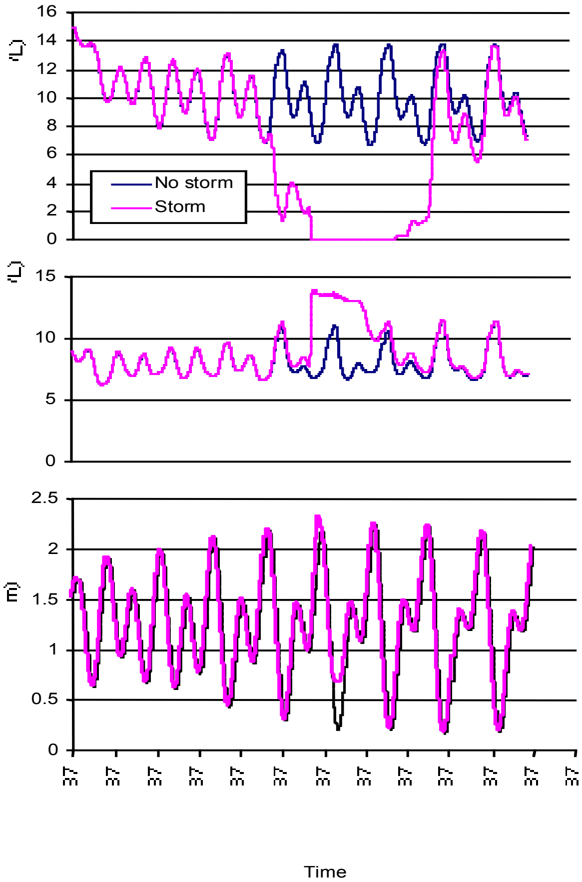

Figure 6. WASP-computed chlorophyll-a, dissolved oxygen, and water depth for storm and non-storm cases in the Ballona Creek estuary.

normal hydrodynamics in the system, increasing the depth from 0.1 to 0.5 m. The storm also affected the water quality and aquatic habitat in the system. Water quality in the Ballona Creek Estuary was controlled by the tides as evidenced by the dissolved oxygen and chlorophyll-a concentrations fluctuating with the tidal level. During the rain event which began Dec. 4, a pulse of highly oxygenated stormwater overwhelmed the tidal forces and washed out any resident algal biomass. Considering the large volume of runoff flow resulting from rain events in this watershed it should be expected that a salt wedge will develop in the estuarine portions of the system due to temperature and salinity differences between the urban runoff and tidal inflow. If a salt wedge forms, then the degree of scouring of algae, suspended solids, and any contaminants could be expected to be less significant.

4.2 Case Study: Emissions Inventory Reduction

In this section, we look at a hypothetical air quality emissions inventory reduction option and evaluate its effect on water quality in order to demonstrate the cross-media utility of the modeling system. For the control case, we have used the 1987 inventory prepared for SCAQS as described by Harley et al. (1993). The hypothetical emissions inventory is based upon the 1997 Air Quality Management Plan (SCAQMD, 1997) which projects a 51% decrease in VOC emissions from 1987 to the year 2000 and a 32.3% decrease in NO_X emissions for the same span of years. These projections are for the Average Annual Day. These emission reduction projections, and a 30% reduction in ammonia emissions, were applied to what we are calling the Year 2000 simulation.

Figure 7 shows the differences in nitrate deposition between using the 1987 and 2000 emissions inventories as input to CIT. For this simulation, we have used the same Dec. 3rd, 1987 wind field for both cases. Reduction in nitrate deposition ranged from 14-18 percent in most grid cells. One should keep in mind that the several large values found over water are for very small mass flux values (see Fig. 4).

The deposition fields produced by the Year

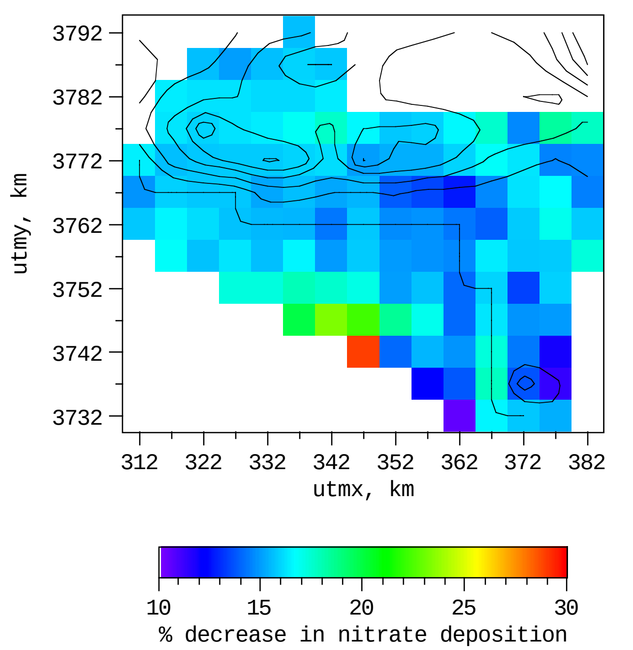

Figure 7. CIT-computed nitrate deposition reduction for Dec. 3, 1987 when replacing the 1987 emissions inventory with the hypothetical Year 2000 inventory.

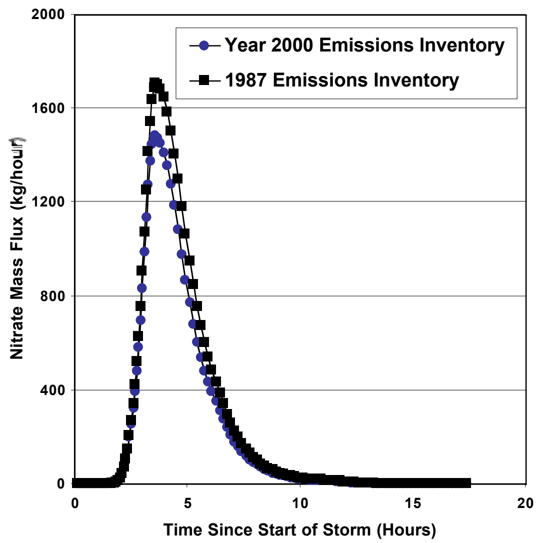

Figure 8. Nitrate mass flux at the Sepulveda Channel outlet (see Fig. 5) for the Dec. 4th rain event using the two different air quality emissions inventories.

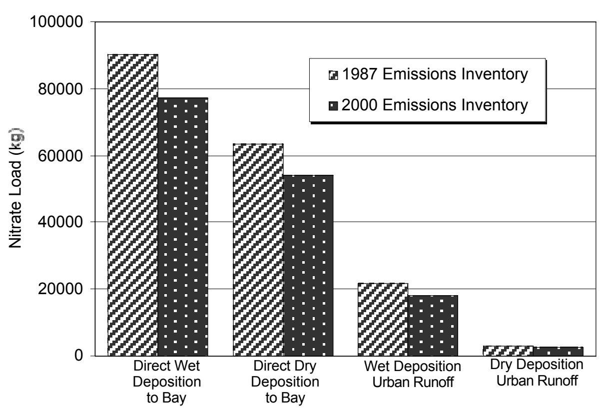

Figure 9. Atmospheric contribution to nitrate loading of Santa Monica Bay broken down into direct wet and dry deposition to the Bay and urban runoff from dry and wet deposition onto Ballona Creek watershed.

2000 emissions inventory was then used as input to the SWMM model. Using the same storm data as described earlier, urban runoff from the sub-catchments was computed and then routed into the storm-sewer network. Figure 8 shows the variation of nitrate mass flux with time at the Sepulveda channel outlet for the 1987 and 2000 emissions inventory cases. This mass flux includes both the nitrate from wet deposition and the "available" dry deposition (i.e., the amount not taken up by plants) that accumulated between rain events (15 days). The peak flux is reduced 15% for the Year 2000 case.

Figure 9 shows the total nitrate load to the Santa Monica Bay computed using the CIT and SWMM models. Results computed using the Year 2000 emissions inventory display a 10-20% reduction in nitrate loading across the board. An interesting feature is that the model results indicate that direct deposition to the Bay overwhelms urban runoff carrying atmospherically-deposited nitrates, even though airborne concentrations of nitrates are relatively small over the Santa Monica Bay. There are several reasons for this result: first, the Bay is about twice as big as the Ballona Creek watershed; second, much of the dry-deposited material on the land surface is taken up by plants and therefore is not available for runoff; and third, from empirical observations the SWMM model assumes that only a fraction of the material deposited onto the ground is entrained by the runoff. The total amount of material dry deposited to the Ballona Creek watershed during the 15 days between rain events was a little over 200,000 kg, so that one can see that most of this material did not find its way into the runoff. As explained in Burian et al. (2000), the assumptions that go into determining the availability of nitrates for runoff are very crude. In addition, the wet deposition has been computed by assuming that all the nitrates in the air are rained out. Hence, one should view the results implied by Fig. 9 with some skepticism.

5. CONCLUSIONS

We have described a set of models that are being used for studying the transport and fate of pollutants through air and water pathways in an urban environment. We have shown results from each of the models in the system and looked at a hypothetical environmental problem that involved linking together air and water quality models.

Our study problem is pushing research development within individual models and in feedback dynamics and interface issues between models. In addition, data availability and validation issues have arisen, namely that long-term data sets are temporally and spatially sparse, while the relatively dense short-term data sets for air and water quality do not coincide in space and time and are few in number.

Our ultimate goal for this project is to link together other models of urban infrastructure and natural systems in order to understand the complex interactions of the urban and natural environments. Such a modeling system could be used for urban planning, sustainability studies, and vulnerability assessment. More information on other work ongoing in this project can be found at http://www-tsa.lanl.gov/tsa4/aquality/urban.html.

Acknowledgements. We wish to thank Grant Heiken for supporting this work as part of the Urban Security Project.

6. REFERENCES

Ambrose, R., T. Wool, J. Martin, “The Water Quality Analysis Simulation Program, WASP5, Part A: Model documentation, Version 5.10.” USEPA, Env. Research Lab., Athens, GA (1993).

Brown, M., S. Burian, T. McPherson, G. Streit, K. Costigan, and B. Greene, “Pollutant transfer through air and water pathways in an urban environment”, *2nd AMS Urban Env. Symp.*, Albuquerque, NM (1998).

Burian, S., T. McPherson, G. Streit, M. Brown, and J. Turin, “Modeling the atmospheric contribution of nitrogen compounds in stormwater runoff”, *11th AMS/AWMA Conf. Appl. Air Poll. Meteor.*, Long Beach, CA (2000).

Costigan K., “Simulation of a winter precipitation event for Los Angeles water quality studies,” AMS 2nd Urban Env. Symp., Albuquerque, NM (1998).

Fisher, D and Oppenheimer, M., "Atmospheric nitrogen deposition and the Chesapeake Bay Estuary." Ambio, 20: 102-108 (1991).

Harley R. A., A. G. Russell, G. J. McRae, G. R. Cass, and J. H. Seinfeld, “Photochemical Modeling of the Southern California Air Quality Study,” *Environ. Sci. Technol.* **27**, 378-388 (1993).

Huber W. and R. Dickinson. "Storm Water Management Model, Version 4: Part A, User's Manual." EPA-600/3-88-001a, USEPA, Washington, DC. (1988).

Jordan T., Correll, D., and Weller, D., "Nonpoint source discharges of nutrients from Piedmont watersheds of Chesapeake Bay." J Amer. Water Resources Assoc., 33(3): 631-645 (1997).

Lawson D., “Southern California Air Quality Study,” JAPCA 40 (1990).

McRae G., W. Goodin and J. Seinfeld. Atmos. Environ. 16, 679-696 (1982).

Pielke R., W. Cotton, R. Walko, C. Tremback, W. Lyons, L. Grasso, M. Nicholls, M. Moran, D. Wesley, T. Lee, and J. Copeland, “A Comprehensive Meteorological Modeling System”, Meteorol. Atmos. Phys. 49, 69-91 (1992).

Russell A., K. McCue, and G. Cass, Environ. Sci. Technol. 22, 263-271 (1988).

Russell A., D. Winner, R. Harley, K. McCue, and G. Cass, "Mathematical modeling and control of the dry deposition flux of nitrogen-containing air pollutants," Environ. Sci. Technol. 27, 2772-2782 (1993).

SCAQMD, 1997. 1997 Air Quality Management Plan.

Solomon P., L. Salmon, T. Fall, and G. Cass, “Spatial and temporal distribution of atmospheric nitric acid and particulate nitrate concentrations in the Los Angeles area,” Environ. Sci. Tech. 26, 1594-1601 (1992).

SMBRP, “Taking the Pulse of the Bay - State of the Bay 1998,” Santa Monica Bay Restoration Project (April 1998).

Suffet, I., J. Froines, E. Ruth, L. Schweitzer, and M. Capangpangan, “Chemical Contaminant Release into Santa Monica Bay: A Pilot Study,” Final Report, Amer. Oceans Campaign (1993).

Stenstrom, M., personal communication (1999).

Wong, K., E. Strecker, and M. Stenstrom, “GIS to estimate storm-water pollutant mass loadings,” J Env. Eng., 737-745 (1997).

Yamada T. and J. Kao, “A modeling study on the fair weather marine boundary layer of the GATE,” J. Atm. Sci. 43, 3186-3199 (1986).